

## From *ab initio* calculation to the prediction of thermodynamic properties of geological properties

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Using atomic site-site potentials to account for the angle-dependent molecular interactions with parameters directly from *ab initio* calculation results, We are able to predict the phase equilibria of CH<sub>4</sub> hydrate and CO<sub>2</sub> hydrate in binary systems over a wide temperature-pressure range (from 243–318 K, and from 10–3000 bar for CH<sub>4</sub> hydrate; from 253–293 K, and from 5–2000 bar for CO<sub>2</sub> hydrate) with accuracy close to experiment. This model is also capable of predicting the cage occupancy and hydration number for CH<sub>4</sub> hydrate and CO<sub>2</sub> hydrate without fitting any experimental data.

In another case of study, we use the *ab initio* potential surface across CO<sub>2</sub>–H<sub>2</sub>O molecules and carried out more than one thousand molecular dynamics simulations of the PVTx properties of the CO<sub>2</sub>–H<sub>2</sub>O mixtures in the temperature–pressure range from 673.15 to 2573.15 K up to 10.0 GPa. Comparison with extensive experimental PVTx data indicates that the simulated results generally agree with experimental data within 2% in density, equivalent to experimental uncertainty. The consistent and stable predictability of the simulation from low to high temperature–pressure and the fact that the molecular dynamics simulation resort to no experimental data but to *ab initio* molecular potential makes us convinced that the simulation results should be reliable up to at least 2573 K and 10 GPa with errors less than 2% in density. The success of these studies validates the predictability of *ab initio* intermolecular potentials for thermodynamic properties of geochemical systems.

## Petrogenetic and metallogenic evolution of the West Cascades arc – A tale of thin crust

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Present-day High Cascades arc magmatism was preceded by ~40 m.y. of nearly co-spatial magmatism represented by the ancestral West Cascades arc. Time-space-composition relations for the West Cascades arc have been synthesized from a new compilation of >4000 geochemical analyses and associated age data. Neither the composition nor distribution of West Cascades magmatism was uniform along the length of ancestral arc through time. Initial (>40-35 Ma) West Cascades magmatism (mostly basalt-basaltic andesite) was focused at the north end of the arc between the present-day locations of Mt. Rainier and the Columbia River. From 35-17 Ma, initial basaltic andesite and andesite magmatism evolved to include dacite and rhyolite; magmatic activity became more voluminous and extended along most of the arc during this time. Between 17-7 Ma magmatism was focused along the arc segment coincident with the northern two thirds of Oregon and returned to more mafic compositions. Subsequent West Cascades magmatism was dominated by basaltic andesite to basalt compositions before the post-4-Ma onset of High Cascades magmatism. Transitional tholeiitic to calc-alkaline compositions dominated early (40 to ~25 Ma) West Cascades eruptive products, whereas younger rocks have a calc-alkaline affinity. Tholeiitic compositions characteristic of the oldest ancestral arc magmas suggest development above thin, immature crust, whereas the younger, calc-alkaline magmas suggest interaction with thicker, more evolved crust. The compositional transition is also reflected in the number and character of mineral deposits associated with the ancestral arc. Mineral deposits in West Cascades are uncommon and most are small relative to other continental arcs, probably reflecting thin, primitive crust that prevailed during most West Cascades magmatism. Low-grade porphyry copper deposits associated with rocks of the West Cascades arc in Washington, north of Mt. St. Helens, may be a consequence of Mesozoic continental crust beneath Washington but not farther south.